PHYSICAL REVIEW
LETTERS

VOLUME 22 | 2 JUNE 1969 | NUMBER 22

# COMPARISON OF THE CALCULATED AND OBSERVED RESONANCES IN THE $e$-H ELASTIC-SCATTERING CHANNEL ABOVE 10.0 eV

S. Ormonde* and J. McEwen*
Quantum Systems, Inc., Albuquerque, New Mexico 87108

and

J. William McGowan†
Gulf General Atomic, Inc., San Diego, California
(Received 21 October 1968; revised manuscript received 16 April 1969)

A wide structure observed experimentally in the elastic cross section for electron–hydrogen-atom scattering below the $n=2$ threshold is analyzed using close-coupling calculations. Good agreement with experiment is found for the six-state approximation.

Recent measurements of the electron–hydrogen-atom elastic-scattering cross section show a rather wide structure immediately below the $n=2$ threshold.[1] This structure has been qualitatively attributed[2] to the $^1D$ and $^1S$ compound states of $H^-$ that have already been partially discussed in the literature, but until this report no comparison between theory and experiment had been made.[3,4] We report here the comparison between theory and experiment wherein the theoretical results were obtained by computing the differential cross section at 90°, averaging over the acceptance angle of 15°, and folding in the energy distribution. We identify the principal compound state of $H^-$ contributing to the structure as the $^1D$ resonance, and we find a substantial agreement between our six-state calculations and experiment.

The theoretical results are based on close coupling calculations using both the three-state ($1s$-$2s$-$2p$) and six-state ($1s$-$2s$-$2p$-$3s$-$3p$-$3d$) eigenfunction expansion.[4] Previous comparisons of different eigenfunction expansions for the lowest lying $^1S$ resonance indicated that potential scattering up to the $n=2$ threshold was reasonably well described by the three-state expansion, but the addition of the higher states was necessary to describe resonance scattering more accurately.[4] In particular, the position of the first $^1S$ resonance was found to be independent of the number of states retained, but the width was decreased by about 5% in using the six-state instead of the three-state expansion. In Fig. 1(a) we show the $^1D$ partial-wave contribution to the total cross section over the resonance region calculated in both the three- and six-state expansions. In contrast to the $^1S$ result quoted, there is in the $^1D$ contribution a shift in the position of the resonance induced by inclusion of the extra closed channels. This shift raised the question of whether it was due to the proximity of the threshold or to the inadequacy of the three-state expansion to describe the higher angular momentum states in the elastic channels. This second alternative would be consistent with a similar effect noted in the inelastic channels below the $n=3$ threshold.[5] The first alternative was eliminated by calculating the position and width of the second $^1S$ resonance which is also close to the $n=2$ threshold. The addition of the higher states had little effect.

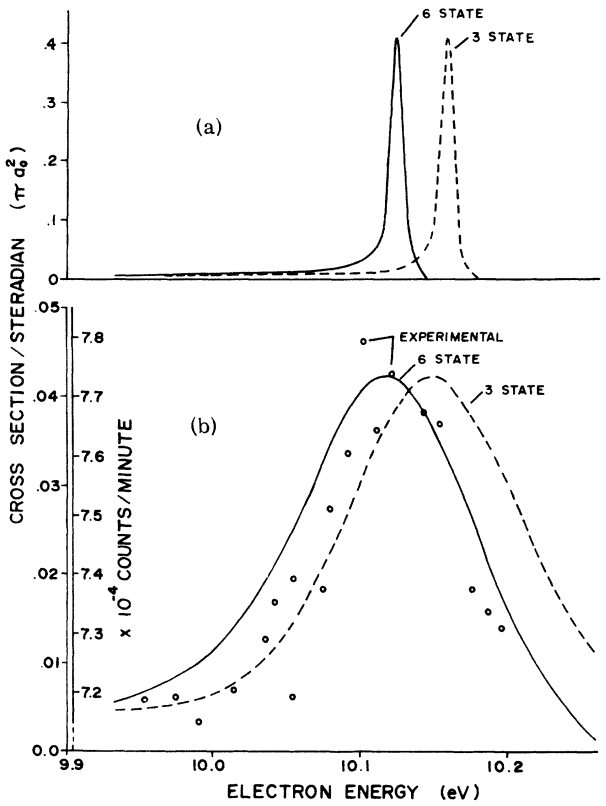


FIG. 1. (a) Close-coupling $^1D$ cross sections over the resonance region. (b) $^1D$ cross sections folded with the resolution of the experimental electron beam. The theoretical calculations correspond to the left-most scale, and the experimental points to the scale on the right. Because the measurements are relative, the results are displayed as shown in order to emphasize the agreement on shape between theory and experiment.

The close coupling $^1D$ differential cross sections calculated at 90° were then averaged over a 15° cone because that was the angle through which the experimentally observed scattered electrons were collected. They were then folded with the resolution of the electron beam used in the experiment (0.08 eV)[1]; this result is shown in Fig. 1(b). A valid comparison with experiment, however, can only be made if the $S$, $P$, and $^3D$ contributions to the cross section are included. The major resonances in these contributions are in $^1S$ and $^3P$ partial waves. The width of the $^1S$ resonance is a factor of 4 smaller than that of the $^1D$ resonance[6] and the $^3P$ parameters are tabulated along with $^1D$ in Table I. Other resonances belonging to these series will be narrower and cannot be expected to contribute anything significant to the final result. The $^{1,3}S$, $^{1,3}P$, and $^3D$ background contributions were included in the differential cross-section calculation at 90°, averaged over the 15° cone, and folded with the experimental beam width as was done with the $^1D$ contribution alone. The calculation was also carried out with the $^1S$ and $^1D$ resonances, including $^{1,3}S$, $^{1,3}P$, and $^{1,3}D$ background phase shifts. At 90° the $P$-wave contribution to the cross section should be zero, so the calculation was repeated with no $P$-wave contributions and no $^1S$ resonance contribution. There was a 1% change in the peak value of the cross section and no change in the position of the peak. In Fig. 2 we show the result of including the $^1S$ and $^1D$ resonances as well as the $^{1,3}S$ and $^{1,3}D$ backgrounds in the calculation. This result is also within 1% of the two results just quoted. This shows conclusively that the dominant contribution to the experimentally observed structure comes from the compound $^1D$ state of the $e$-H system. The absolute scale for the experimental points was obtained by normal-

Table I. Peak position of the $^1D$ cross section, and position and width of the theoretical $^1D$ and $^3P$ resonances, all in eV.

| | $^1D$ resonance alone | | $^1D$, $^1S$ resonance + background | |
|---|---|---|---|---|
| | Unfolded | Folded | Unfolded | Folded |
| 3 state | 10.156 | 10.149 | 10.163 | 10.183 |
| 6 state | 10.122 | 10.115 | 10.129 | 10.149 |
| Expt.[a] | ... | ... | ... | 10.13 ± 0.015 |

| | $^3P$ | | $^1D$ | |
|---|---|---|---|---|
| | $E_R$ | $\Gamma$ | $E_R$ | $\Gamma$ |
| 3 state | 10.194 | 0.0008 | 10.160 | 0.0078 |
| 6 state | 10.190 | 0.0002 | 10.126 | 0.0088 |

[a]See Ref. 1.

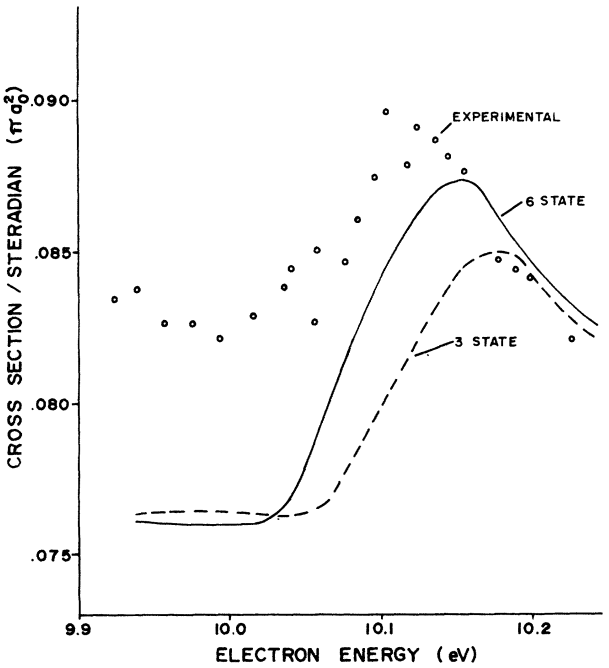


FIG. 2. Cross-section calculation at 90° including $^1D$, $^1S$ resonances and $^{1,3}S$, $^{1,3}D$ background averaged over 15° acceptance angle and folded with the resolution of the experimental electron beam. The experimental points are here normalized using the scale obtained by normalizing the measured differential scattering data in the region below the lowest $^1S$ resonance to the calculated cross section in that region.

izing the measured differential scattering data in the region below the lowest (i.e., at 9.56 eV) $^1S$ resonance to the calculated cross section using the best available phase shifts.[2] The effect of including the background in the folded and unfolded cross sections is summarized in Table I.

Because of the energy spread of the bombarding electrons, the measurements for energies nominally below $n = 2$ contain some information from above $n = 2$. As it is difficult to calculate the elastic-scattering phase shifts through and immediately above the inelastic threshold and since the resonance lies so close to the $n = 2$ threshold, comparison with experiment could be carried out only if some assumptions were made about the values of the phase shifts immediately above and below the $n = 2$ threshold. Consequently, for the folded cross-section calculations we extrapolated all the phase shifts across the threshold.

In summary, we have shown that in the elastic-scattering channel immediately below $n = 2$, the description by the close-coupling approximation of the $D$ states of $H^-$ depends on whether the $n = 3$ states of the neutral atom are included in the eigenfunction expansion. We have also shown that the $^1D$ compound state of $H^-$ is the dominant contribution to the experimentally observed structure and we would like to suggest that this be verified by a measurement of the differential cross section at 54 $\frac{1}{2}$°, the angle at which the $D$ contribution is zero.

We would like to acknowledge here the careful and patient help of Miss K. Thomas throughout these calculations.

---

*Work supported by the Defense Atomic Support Agency through the Air Force Weapons Laboratory, Kirtland Air Force Base, N. Mex., Contract No. AF29(601)-68-C-0052 with Quantum Systems, Inc., Albuquerque, N. Mex.

†Work supported by National Aeronautics and Space Administration under Contract No. NAS 5-11025 with Gulf General Atomic, Inc.

[1]J. William McGowan, E. M. Clarke, and E. K. Curley, Phys. Rev. Letters 15, 917 (1965), and 17, 66(E) (1966).

[2]J. William McGowan, Phys. Rev. 156, 165 (1957).

[3]J. C. Y. Chen, Phys. Rev. 156, 150 (1967).

[4]P. G. Burke, S. Ormonde, and W. Whitaker, Proc. Phys. Soc. (London) 92, 317 (1967).

[5]J. W. McGowan and J. Williams, Bull. Am. Phys. Soc. 13, 896 (1968), and in Proceedings of the Arnold Sommerfeld Centennial Memorial Meeting and Symposium on Physics of One- and Two-Electron Atoms, Munich, Germany, 9-14 September 1968 (North-Holland Publishing Company, Amsterdam, The Netherlands, to be published).

[6]P. G. Burke, in Proceedings of the Fifth International Conference on the Physics of Electronic and Atomic Collisions, Leningrad, 1967, edited by L. M. Branscomb (Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colo., 1968), p. 128.